NUMERICAL ANALYSIS OF A MASS SEPARATOR

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Abstract: The presented work investigates numerical approach to the movement of charged particles. Custom model describing electromagnetic forces on particles was created and implemented into ANSYS FLUENT. This model was then used for a simulation of a simplified version of a mass separator. Results were then compared to the theoretical results which were closely comparable.

Keywords: ANSYS FLUENT, discrete phase model, charged particles, mass separator

1 INTRODUCTION

Mass separator is a device that separates ions based on their mass in relation to their charge. By selecting right parameters, it is possible to define which ions will pass through the separator. This means it can be used for many applications such as: mass spectrometry, ion implantation or ion deposition. Usually these devices have similar base composition which consists of ion source, separator and final component which is for example a detector for mass spectrometry or a substrate for ion implantation and deposition. [1] Numerical simulations act as great tool for investigating processes or devices utilizing charged particles as it is sometimes hard to study them experimentally. Another advantage of numerical simulations is in designing and optimizing where they speed up this process.

2 NUMERICAL MODEL

For these simulations, ANSYS FLUENT was used. It is a complex CFD software which uses finite volume method to numerically calculate partial differential equations. Euler-Lagrange approach is used in Discrete Phase Model (DPM), in which fluid phase is treated as a continuum by solving Navier-Stokes equations while the discrete phase is solved by tracking individual particles through the computational domain. With this approach, phases can exchange energy, momentum and mass between each other. This model can be significantly simplified by neglecting particle-particle collisions. This simplification is valid for low volume fraction of particles, so the particle trajectories are computed individually at specified intervals during the fluid phase calculation. Basic equation for the movement of a particle can be described as [2]:

$$\frac{d\boldsymbol{p}}{dt} = m\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F} \tag{1}$$

Where $\boldsymbol{p}$ is momentum [kg·m·s^{-1}], t is time [s], m is mass [kg], $\boldsymbol{v}$ is velocity vector [m·s^{-1}], $\boldsymbol{F}$ is acting force vector [N].

However, without any modifications ANSYS FLUENT is not able to fully model the movement of charged particles in vacuum. Although ANSYS FLUENT has in-built Electric Potential model and Magnetohydrodynamic model, these models are incomplete and are not capable of modelling a movement of charged particles in electromagnetic field. Electric potential model solves only electric field and Magnetohydrodynamic model cannot model effect of magnetic field on a charged par-

ticle in a non-conductive medium. For this reason, new custom model was created and implemented into ANSYS FLUENT. It was written through User Defined Scalars (UDSs) and User Defined Functions (UDFs). Four UDSs were created: one for electric potential and three for each component of magnetic vector potential. For every UDS, a transport equation is solved. General transport equation can be described as [3]:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \left(\boldsymbol{v}\phi - \Gamma \nabla \phi \right) = S_\phi \tag{2}$$

Where ϕ is a general scalar quantity, Γ is a diffusion coefficient, S_ϕ is a source term.

Then through the UDF, source terms for magnetic vector potential and electric potential were added. As the external fields are constant, only static equations were implemented. Main equations of this models are described as:

$$\nabla \cdot (-\varepsilon \nabla \varphi) = \rho \tag{3}$$

$$\nabla \cdot (-\frac{1}{\mu} \nabla \boldsymbol{A}) = \boldsymbol{j} \tag{4}$$

$$\boldsymbol{j} = -\sigma \nabla \varphi \tag{5}$$

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{6}$$

Where ε is permittivity [F·m^{-1}], φ is electric potential [V], ρ is charge density [C·m^{-3}], μ is permeability [H·m^{-1}], $\boldsymbol{A}$ is magnetic vector potential [V·s·m^{-1}], $\boldsymbol{j}$ is current density vector [A·m^{-2}], σ is electric conductivity [S·m^{-1}], $\boldsymbol{B}$ is vector of magnetic flux density [T].

Equations 3 and 4 are transport equations and are calculated directly. Other equations are calculated from the transport equations and are stored in User Defined Memory.

Another UDF was used to model the effects of electromagnetic field on charged particles. These effects are described as Lorentz force:

$$\boldsymbol{F}_L = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \tag{7}$$

Where q is electric charge [C], $\boldsymbol{E}$ is electric intensity vector [V·m^{-1}].

FLUENT doesn't include a drag law suitable for the movement of particles in a vacuum. Due to a simplification it was assumed that there are no interactions between fluid and particles. This assumption was also implemented through a UDF.

So, the final form of equation that describes the movement of charged particles is:

$$m\frac{d\boldsymbol{v}}{dt} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \tag{2}$$

3 ANALYSIS

Numerical model presented above was tested on a simplified geometry of a mass separator. The analyses studied a movement of three types of charged particles - aluminium, copper and gold, so the differences, based on their mass, could be investigated. It was assumed that all of the ions were already created with a zero initial velocity and had charge number of 1. The parameters of the mass separator were chosen so that copper ions would pass through. Whole process was divided into few parts. First, the ion acceleration is studied and then later, a simplified ion accelerator is combined with a separation region. As particles have no interaction with a continuum medium, it was assumed that there was no flow in the domain and only electromagnetic field and particle movement were calculated.

3.1 MATERIAL PROPERTIES

In the DPM, parameters of the discrete phase are calculated from macroscopic properties of materials. However, this is not a valid assumption for single atoms, because in macroscopic matter there is an empty space between atoms which results in lower macroscopic density. For this reason, new parameters were calculated from atomic radius and relative atomic mass as shown in Table 1.

Table 1: Material properties

Material	Macroscopic density [kg·m^{-3}]	Radius [pm]	Relative atomic mass [-]	New atomic mass [kg]	New density [kg·m^{-3}]
Aluminium	2700	143	26,9815	4,482e-26	3658,78
Copper	8940	128	63,546	1,056e-25	12015
Gold	19000	135	196,967	3,272e-25	31748,5

3.2 ION ACCELERATION

Ions as charged particles can be accelerated by electric field. At the beginning of this process, particles have zero kinetic energy and maximal potential energy then gradually they are accelerated, and potential energy is transferred into kinetic. Maximum velocity can be derived from:

$$\frac{1}{2}mv^2 = qU \tag{9}$$

$$v = \sqrt{\frac{2qU}{m}} \tag{10}$$

As a first step, analysis of a simplified ion accelerator was carried out. The intensity of accelerating electric field was set to 1000 V/m. The geometry consisted of three chambers which were divided by two apertures with a diameter of 5 mm. Left chamber functioned as a starting point for particles, and a boundary condition of 100 V was set there. Boundary condition of 0 V was set on the right aperture. This setup caused the acceleration of particles in the middle chamber.

Table 2: Comparison of velocities

Material	Theoretical Velocity [m·s^{-1}]	Calculated Velocity [m·s^{-1}]
Aluminium	26878,34	26733,70
Copper	17510,82	17419,93
Gold	9947,91	9920,54

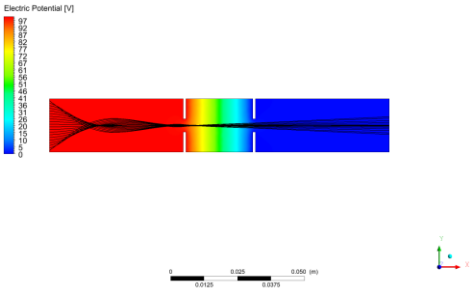

Figure 1: Accelerating electric field

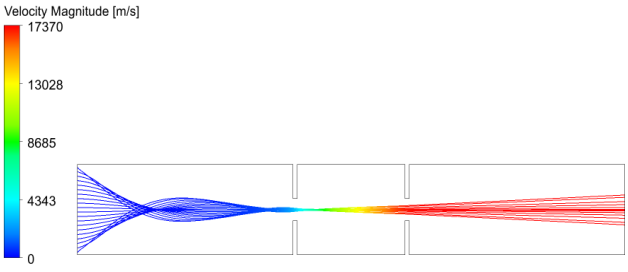

Figure 2: Velocity of charged particles

3.3 SEPARATION

Separation region consist of constant magnetic field which is perpendicular to the velocity of particles. Magnetic fields exert force on particles, and they start to follow circular trajectory. The radius R_k is described as:

$$R_k = \frac{mv}{qB} = \frac{1}{B}\sqrt{\frac{2qU}{m}} \tag{11}$$

The analyses of two different mass spectrometer arrangements were carried out.

Both arrangements consist of ion accelerator and a separation region, but they differ in the shape of the separation region.

First arrangement is characterized by a half circle trajectory of charged particles. The constant magnetic field was selected from the equation 11, in which the desired radius of copper ions was set to 50,50 mm. Magnitude of magnetic flux was set to 0, 227227 T. As expected, aluminium ions are deflected more which results in smaller radius, and heavier gold ions are deflected less which results in bigger radius. Results from this simulation were compared with theoretical values in Table 3.

Table 3: Comparison of radii

Material	Theoretical radius [mm]	Calculated radius [mm]
Aluminium	34,53	33,488
Copper	50,50	51,24
Gold	89,89	89

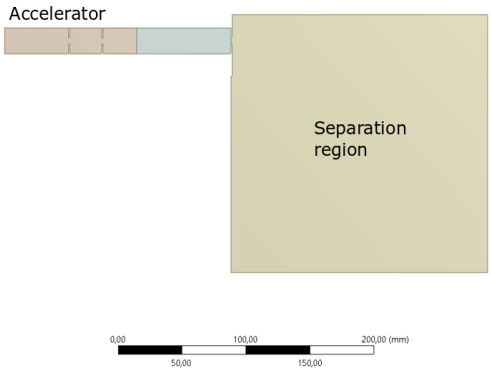

Figure 3: Geometry of first mass separator

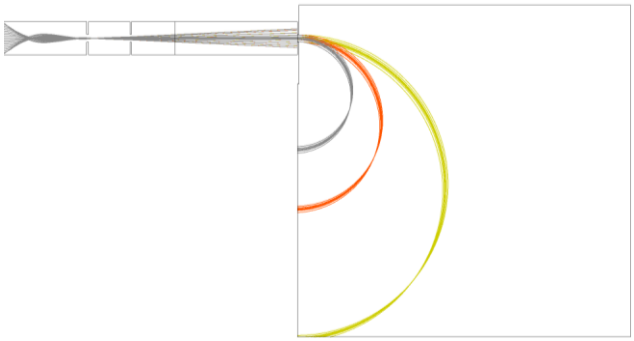

Figure 4: Trajectories of aluminium (gray), copper (orange) and gold (yellow) ions

Second arrangement of mass spectrometer is characterized by separation region in a shape of quarter circle. The region has a radius of 50 mm, and so the magnetic flux density was calculated so the copper ions follow the desired trajectory. Similar to the first example, lighter aluminium ions bend too much and heavier gold ions bend too little so they can't pass the separator.

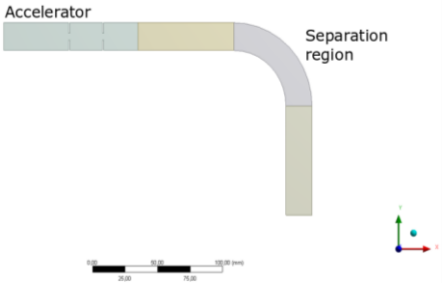

Figure 5 Geometry of second mass separator

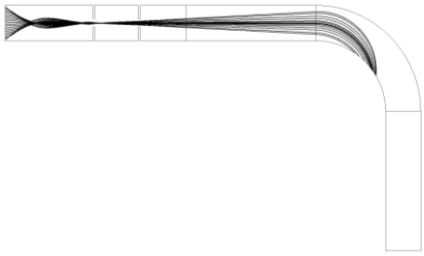

Figure 6 Trajectories of aluminium ions

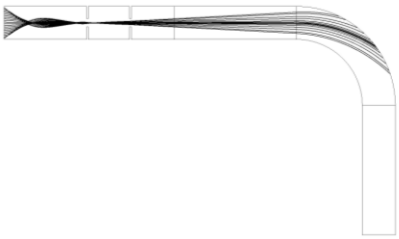

Figure 7 Trajectories of gold ions

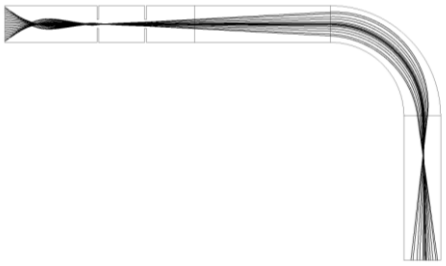

Figure 8 Trajectories of copper ions

4 CONCLUSION

The movement of charged particles was investigated using CFD software ANSYS FLUENT. While FLUENT has in-built Discrete Phase Model and Magnetohydrodynamic model, these models are insufficient for studying such movement. For this reason, a custom numerical model was created and implemented into FLUENT. This model was then applied to a simplified version of a mass separator. Results gathered from simulation were compared to theoretical results. These results were closely comparable and so this model might be used as an optimization tools for mass spectrometry or ion deposition or implantation.

ACKNOWLEDGEMENT

This work was supported by the BUT specific research programme (project No. FEKT-S-17-4595).

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